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Examples and Notes on Multiple Integration

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EXAMPLES AND NOTES ON MULTIPLE INTEGRATION

by

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When using a numerical method of approximating the value of the definite integral $\int_a^b f(x)dx$, it is of course very important that one knows the character of the integrand; does $f(x)$ or its derivative have any singularities in the closed interval $[a,b]$, and, if so, what type of singularities are present? The answers to these questions will determine the type of quadrature formula which should be used.

In the case of a one-dimensional integral with a reasonably simple integrand, one can usually determine fairly easily whether or not a singularity is present and - perhaps with more difficulty - the character of the singularity. Sometimes the singularity may be removed by a change of variables, so that a standard non-singular type quadrature formula may be used. In other cases one uses a generalized Gauss formula (or similar formula with other spacing) which has been derived using a proper weighting function for the singularity in question.

In the case of two-dimensional integrals, it is easier to be misled by one's intuition. With the advent of high-speed digital computers, it has become the tendency to ask for general computer programs which will integrate any "reasonable" function. Multiple integrals are usually treated as repeated simple integrals, (so that one-dimensional quadrature formulas are used two or more times). It is the purpose of these notes to give some simple examples of multiple integrals which show some of the difficulties which may arise. Also some formulas will be given to use on singular integrals of the types

$$\int_0^h \int_0^h \frac{F(x,y)}{\sqrt{x^2 + y^2}} dxdy$$

and

$$\int_0^h \int_0^h \ln \sqrt{x^2 + y^2}\, F(x,y)\, dxdy$$

which occur from time to time in physical problems. In the three appendices, the formulas discussed in the text are collected for ready reference. No formal expressions for error terms associated with the formulas of Appendix II and Appendix III are given.

§1. Examples in which the integrand is non-singular.

Example 1: Consider $\iint_A F(x,y)dxdy$, where $F(x,y) \equiv 1$ and where A is the first quadrant area enclosed by the curve $y = 1 - x^2$. (See Figure 1).

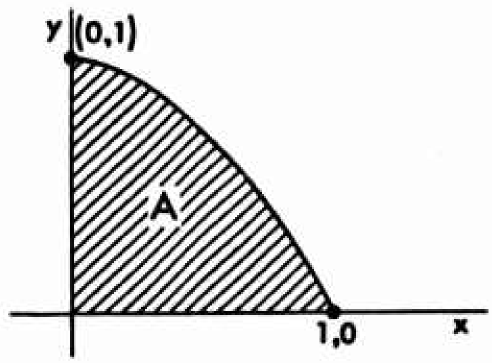

Figure 1

The multiple integral may be written as an iterated integral in either of two ways:

$$I = \int_0^1 \left[\int_0^{\sqrt{1-y}} dx \right] dy \tag{1.1}$$

$$I = \int_0^1 \left[\int_0^{1-x^2} dy \right] dx \tag{1.2}$$

With either form, one can easily perform the integrations analytically and arrive at the exact answer $I = 2/3$. Since $F(x,y)$ is such a smooth function (identically 1), one might suspect at first sight that (1.1) or (1.2) could be evaluated quite well by use of Simpson's rule. This was actually programmed on a machine. In both cases the inner integrals were evaluated by using a 5-point Simpson formula. The second integration was also performed using Simpson's rule, and it was tried several times using different integration step lengths. The results are given in Table 1.

Number of Points Used In Outer Integration Formula	Numerical Result Problem (1.1)	Numerical Result Problem (1.2)
5	.65652626	.66666668
9	.66307927	.66666667
17	.66539809	.66666676
33	.66621795	.66666672
65	.66650784	.66666688
129	.66660944	.66666813
257	.66664446	.66666923

Table I: Results (using Simpson's Rule) to evaluate integral in (1.1) and (1.2)

<u>Comments on the results</u>: It is seen that for problem (1.2) Simpson's rule gives very close to the correct answer 2/3. As more points are taken, the results do get poorer, but this is caused entirely by round-

off error.

In the case of problem (1.1), Simpson's rule gives results which are quite poor. The results do get better as more points are taken, but if five-place accuracy were desired, many more than the $257 \times 5 = 1275$ points would be required; it is obvious by looking at the differences, caused by round-off in problem (1.2) that round-off errors would also "take over" in problem (1.1) before five-figure accuracy could be attained.

With such a simple example, it is quite readily seen <u>why</u> the order of integration makes so much difference. If the inner integration were done analytically, equation (1.1) would become

$$I = \int_0^1 \sqrt{1 - y}\, dy \tag{1.3}$$

while (1.2) would become

$$I = \int_0^1 (1 - x^2) dx. \tag{1.4}$$

Theoretically, (i.e., except for round-off), Simpson's rule should give exact results for the problem of integrating the polynomial $G(x) \equiv 1 - x^2$ over the interval $[0,1]$. On the other hand, the function $H(y) \equiv \sqrt{1 - y}$ may not be approximated very accurately by portions of cubic polynomials (because it has an infinite slope at $y = 1$). Simpson's rule should not be used for such a quadrature; instead a special formula should be used which takes into account the nature of the singularity in $H'(y)$.

<u>Example 2</u>. Consider the integral

$$J = \int_{-1}^{1} \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} \left\{ \frac{t^2}{\sqrt{t^2 + x^2}} + \sqrt{t^2 + x^2} \right\} dtdx. \tag{1.5}$$

Geometrically, the symmetric, non-negative integrand is being integrated over a circle of radius 1. The integration is easily performed analytically, and it is found that $J = \pi$. If one considers this as a repeated simple integral, and if a twelve-point Gauss quadrature formula is used in the intervals $[-\sqrt{1 - x_j^2}, \sqrt{1 - x_j^2}], j = 1,2,\ldots,12$ for the inner integrations and in the interval $[-1,1]$ for the outer integration (so that the integrand has been evaluated at 144 points in all), the result 3.1440 is obtained; the error is + .0024. If thirteen-point Gauss formulas are used (so the integrand has been evaluated 169 times in all), the result 3.1379 is obtained; the error is - .0037.

One might surmise that a reason for the very inaccurate results might be that the integration with respect to t has not been done very accurately when x is close to zero. For example, when $x = 0$, it is desired to integrate $|2t|$ which has a discontinuity in the derivative when $t = 0$. Thus, one expects better results if he evaluates numerically

$$2 \int_{0}^{\sqrt{1-x^2}} \left\{ \frac{t^2}{\sqrt{t^2 + x^2}} + \sqrt{t^2 + x^2} \right\} dt \tag{1.6}$$

instead of

$$\int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} \left\{ \frac{t^2}{\sqrt{t^2 + x^2}} + \sqrt{t^2 + x^2} \right\} dt.$$

If six-point Gauss formulas are used for the integrals (1.6), (equivalent again to the use of 144 points over the whole circle), the final result is 3.1437. The error is now +.0021 (as opposed to +.0024 for the 144 point case before), so the error is still more than expected for the integration of "smooth" functions.

Much more accurate results are obtained if one uses the ordinary Gauss quadrature formulas for performing the t integration and then uses the generalized Gauss formula

$$\int_{-1}^{1} \sqrt{1 - x^2}\, f(x)dx = H_1 f(x_1) + H_2 f(x_2) + \cdots + H_{12} f(x_{12}) \qquad (1.7)$$

for the outer quadrature. Here $x_i = \cos \frac{i\pi}{13}$ and $H_i = \frac{\pi}{13} \sin^2 \frac{i\pi}{13}$ for $i = 1,2,3,\ldots,12$. The final result using this formula is $J \triangleq 3.141630$. The error is only $+.000037$.

Comments on the results: It is often stated that if a double integration problem is symmetric with respect to the two independent variables, one should "treat both variables the same". Then why does the use of ordinary Gauss integration in both directions yield such poor results, and why are results improved so much by using a different formula for the x integration? The answer presents itself when the t integration is actually performed analytically. The result is

$$\int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} \left\{ \frac{t^2}{\sqrt{t^2 + x^2}} + \sqrt{t^2 + x^2} \right\} dt = 2\sqrt{1 - x^2}.$$

Thus we now wish to evaluate $2\int_{-1}^{1}\sqrt{1-x^2}\,dx$, the integrand of which has infinite slopes at $x = \pm 1$. The twelve-point ordinary Gauss formula gave better than four-place accuracy when the t integrations were performed, and the results were of course good approximations to $\sqrt{1-x^2}$. The generalized Gauss formula will evaluate $\int_{-1}^{1}\sqrt{1-x^2}\,dx$ exactly, so it does a good job of integrating the "good approximation" to $\sqrt{1-x^2}$.

Hence, for a symmetric problem, it is often not really possible or desirable to treat both variables "the same" when multiple integration is performed by iterated use of one-dimensional formulas. The choice of a particular variable, with respect to which one integrates first, ruins the symmetry of the problem. (These remarks do not apply if the region of integration is a rectangle.)

§2. Singular integrals of the type $I = \int_{-a}^{a}\int_{-a}^{a} \frac{F(x,y)}{\sqrt{x^2+y^2}}\,dxdy.$ (2.1)

Here it will be assumed that $F(x,y)$ is analytic in the square $-a \leq x,\ y \leq a$ and that $F(0,0) \neq 0$. The difficulties illustrated in §1 with problems in which the original integrand was always finite and continuous should lead one to expect that even more care is necessary in the use of numerical methods when the integrand is infinite at some point.

Theoretically, if $y \neq 0$, the integration with respect to x could be carried out with a standard non-singular formula like Simpson's rule. This would give an approximation for

$$G(y) = \int_{-a}^{a} \frac{F(x,y)}{\sqrt{x^2+y^2}}\,dx.$$

Since $F(x,y)$ is analytic in $-a \leq x \leq a$, $-a \leq y \leq a$, it may be expanded in a Taylor series (with respect to x), so that

$$F(x,y) - F(0,y) - xF_x(0,y) = \frac{x^2}{2!}\{F_{xx}(0,y) + \frac{x}{3} F_{xxx}(0,y) + \cdots\} = \frac{x^2}{2!} H(x,y),$$

where $H(x,y)$ will also be analytic in the square. Assuming still that $y \neq 0$, $G(y)$ may then be written

$$G(y) = F(0,y) \int_{-a}^{a} \frac{dx}{\sqrt{x^2 + y^2}} + F_x(0,y) \int_{-a}^{a} \frac{xdx}{\sqrt{x^2 + y^2}} + \frac{1}{2!} \int_{-a}^{a} \frac{x^2 H(x,y)}{\sqrt{x^2 + y^2}} dx \quad (2.2)$$

or

$$G(y) = F(0,y) \ln\left[\frac{\sqrt{y^2 + a^2} + a}{\sqrt{y^2 + a^2} - a}\right] + \frac{1}{2!} \int_{-a}^{a} \frac{x^2 H(x,y)}{\sqrt{x^2 + y^2}} dx, \quad (2.3)$$

(since the second integral in (2.2) is zero because the integrand is an odd function of x).

The integral in (2.3) is obviously a continuous function of y which will approach a finite limit when $y \to 0$. The first term in (2.3) is also a continuous function of y if $y \neq 0$. But at $y = 0$ this term is logarithmically singular. That is, (since $F(0,0) = \text{constant} \neq 0$),

$$\lim_{y \to 0} \frac{\ln(\sqrt{y^2 + a^2} + a) - \ln(\sqrt{y^2 + a^2} - a)}{\ln|y|} F(0,y)$$

$$= \lim_{y \to 0} \frac{y^2}{\sqrt{y^2 + a^2}}\left[\frac{1}{\sqrt{y^2 + a^2} + a} - \frac{1}{\sqrt{y^2 + a^2} - a}\right] F(0,0)$$

$$= -2F(0,0).$$

Thus $G(y)$ may be written in the form $g(y) \ln|y|$, where $g(y)$ will remain finite throughout $[-a,a]$ if $0 < a < 1$. The problem of performing the cubature of (2.1) has now been reduced to that of performing the two quadratures

$$g(y) = \frac{1}{\ln|y|} \int_{-a}^{a} \frac{F(x,y)}{\sqrt{x^2 + y^2}} dx \qquad (2.4)$$

and

$$I = \int_{-a}^{a} \ln|y| \; g(y) dy. \qquad (2.5)$$

Theoretically, for example, the standard Gauss formula or Simpson's rule could be used to approximate (2.4) when $y \neq 0$. A generalized Gauss formula with weighting function $\ln|y|$ may then be used to approximate (2.5). (For such a formula, see Appendix I). Methods of this type have been used successfully, but here also it is easy to overlook some difficulty which will cause large errors in the result. Consider the special example:

<u>Example 3</u>: $$I_3 = \int_0^1 \int_0^1 \frac{4 + x^2 + y^2}{\sqrt{x^2 + y^2}} dxdy.$$

This integral is essentially of the type (2.1). Since the integrand is symmetric in x and y the two lower limits were taken as zero. Equations (2.5) and (2.4) for this problem would be

$$I_3 = \int_0^1 \ln|y| \; g(y) dy \qquad (2.6)$$

where

$$g(y) = \frac{1}{\ln|y|} \int_0^1 \frac{4 + x^2 + y^2}{\sqrt{x^2 + y^2}}\, dx. \tag{2.7}$$

The four-point generalized Gauss formula

$$I_3 \triangleq H_1 g(y_1) + H_2 g(y_2) + H_3 g(y_3) + H_4 g(y_4)$$

where

$H_1 = -.383464068$ $\quad y_1 = .041448480$

$H_2 = -.386875318$ $\quad y_2 = .245274914$

$H_3 = -.190435127$ $\quad y_3 = .556165454$

$H_4 = -.0392254 87$ $\quad y_4 = .848982395,$

was used to evaluate the integral in (2.6). (The necessary values of $g(y)$ were obtained previously by using an ordinary four-point Gauss formula applied to the integral of (2.7)). The resulting approximate value for I_3 was 7.58863. The integral I_3 may of course be evaluated analytically, and the result is

$$I = \tfrac{1}{3}\{25 \ln(1 + \sqrt{2}) + \sqrt{2}\} \triangleq 7.816186.$$

The approximate result was too low by about 0.23. If we had not worried about the singularity at all, and had merely used the regular four-point Gauss formula for both the x and y integrations, the result would have been 7.7219, which is too low by only about 0.09.

Comments on the results: The question, of course, is why better results are obtained when one ignores the presence of the singularity completely than if formulas (2.6) and (2.7) are used. The main reason is that in"taking care of" the singularity at $y = 0$, a new singularity was introduced at $y = 1$. When using a generalized Gauss formula to evaluate (2.6), it is assumed that $g(y)$ may be approximated reasonably well by a polynomial. However, equation (2.7) shows that $g(1) = \infty$, so the generalized Gauss formula should not have been used to evaluate (2.6); to use it was a definite error in reasoning. The example was given here however to emphasize that such errors will often not show up when the problem is placed on the machine unless the exact answer is known.

The integral I_3 could have been approximated better by treating a smaller region about the singularity as a singular problem and by using standard quadrature formulas in the region away from the singularity. This correct use of formulas analogous to (2.6) and (2.7) is shown in the evaluation of the integrand of Example 3 over a smaller region:

<u>Example 4:</u> $$I_4 = \int_0^{\frac{1}{4}} \int_0^{\frac{1}{4}} \frac{4 + x^2 + y^2}{\sqrt{x^2 + y^2}} \, dx dy.$$

This integral may be evaluated exactly and the result is

$$I_4 = \frac{1}{192}[\sqrt{2} + 385 \ln(1 + \sqrt{2})] \doteq 1.7747034.$$

If the singularity is ignored and an ordinary four-point Gauss formula is used, for both x and y integrations, the resulting value is 1.7511 which is too low by about .0236.

If one desires to perform the cubature as an iterated quadrature (but making use of the fact that the integrand determined by the inner integral has a logarithmic singularity at $y = 0$), the specific formula will be

$$I_4 = \int_0^{\frac{1}{4}} \ln y \; g(y)dy, \tag{2.8}$$

where

$$g(y) = \frac{1}{\ln y} \int_0^{\frac{1}{4}} \frac{4 + x^2 + y^2}{\sqrt{x^2 + y^2}} dx. \tag{2.9}$$

The generalized four-point Gauss formula needed for this problem is of the form

$$\int_0^{\frac{1}{4}} \ln y \; g(y)dy = H_1 g(y_1) + H_2 g(y_2) + H_3 g(y_3) + H_4 g(y_4).$$

The abscissas y_i and the weights H_i are given in the table of Appendix I. Using this formula (and using ordinary four-point Gauss quadrature formulas for approximating each functional value $g(y_i)$), one obtains the value 1.7728 for I_4, which is only in error by about 0.0019.

<u>Comments on the results</u>: The fact that the error 0.0019 (incurred when the presence of the singularity is considered) is only about eight percent of that incurred when the singularity is ignored is encouraging. However, the more accurate method is also subject to criticism. Should the ordinary Gauss formula be used to evaluate (2.9) for the various desired values of y? It is true that for $y \neq 0$ there is no singular point in $0 \leq x \leq \frac{1}{4}$; but as y becomes

very small the function

$$\frac{4 + x^2 + y^2}{\sqrt{x^2 + y^2}}$$

begins to have a graph whose shape is more like that of the function $\frac{4 + x^2}{x}$. Thus numerical results assuming

$$\frac{4 + x^2 + y^2}{\sqrt{x^2 + y^2}}$$

may be approximated by a polynomial in $0 \leq x \leq \frac{1}{4}$ are not very good if y is very close to zero. It would seem that a similar criticism would probably apply to any method of evaluating the singular double integral by an iterated numerical quadrature.

The other possibility is to set up a single two-dimensional formula for numerical integration of

$$I = \int_0^h \int_0^h \frac{F(x,y)}{\sqrt{x^2 + y^2}} dxdy, \tag{2.10}$$

(where $F(x,y)$ is assumed to be analytic in $0 \leq x \leq h$, $0 \leq y \leq h$, and where $F(0,0) \neq 0$). An extremely simple symmetrical formula of this type is of the form

$$I = a\, F(0,0) + b(F(0,h) + F(h,0)) + c\, F(h,h), \tag{2.11}$$

where the coefficients $a, b,$ and c are determined (by the method of undetermined coefficients) so that the formula is exact if F is any polynomial which is linear in both the x-and-y directions. That is, formula (2.11) is to be exact if $F(x,y) = c_1 + c_2x + c_3y + c_4xy$.

Since the last function is linear, it is only necessary to require that formula (2.11) be exact if $F(x,y) = 1$, if $F(x,y) = x$, if $F(x,y) = y$, and if $F(x,y) = xy$. If $F(x,y) = 1$, the requirement is

$$a + 2b + c = \int_0^h \int_0^h \frac{dxdy}{\sqrt{x^2 + y^2}} = 2h \ln(\sqrt{2} + 1). \qquad (2.11a)$$

If $F(x,y) = x$, one obtains

$$hb + hc = \int_0^h \int_0^h \frac{x\, dxdy}{\sqrt{x^2 + y^2}} = \frac{1}{2} h^2[\sqrt{2} - 1 + \ln(\sqrt{2} + 1)]. \qquad (2.11b)$$

If $F(x,y) = xy$, one obtains

$$h^2 c = \int_0^h \int_0^h \frac{xy\, dxdy}{\sqrt{x^2 + y^2}} = \frac{2}{3} h^3(\sqrt{2} - 1). \qquad (2.11c)$$

If $F(x,y) = y$, because of symmetry the same equation is obtained as was obtained when $F(x,y) = x$. Solving for $c, b,$ and a,

$$c = \frac{2}{3} h(\sqrt{2} - 1)$$

$$a = 2b = \frac{1}{3} h[3 \ln(1 + \sqrt{2}) - \sqrt{2} + 1].$$

Hence, formula (2.11) may be conveniently written

$$I = h[.276142375\, F(h,h) + .371651200(F(0,h) + 2F(0,0) + F(h,0))]. \qquad (2.12)$$

In a similar manner, a symmetrical nine-point formula of the type

$$I = a\, F(0,0) + b[F(0,\tfrac{h}{2}) + F(\tfrac{h}{2},0)] + c[F(0,h) + F(h,0)]$$
$$+ d[F(\tfrac{h}{2},h) + F(h,\tfrac{h}{2})] + e\, F(\tfrac{h}{2},\tfrac{h}{2}) + g\, F(h,h) \qquad (2.13)$$

may be obtained, which will be exact for any polynomial of the form

$$F(x,y) = c_0 + c_1x + c_2y + c_3xy + c_4x^2 + c_5y^2 + c_6x^2y + c_7xy^2 + c_8x^2y^2.$$

The coefficients turn out to be

$$a = \frac{h}{30}[11 \ln(\sqrt{2} + 1) - \sqrt{2}] \triangleq .276029863h$$

$$b = \frac{h}{30}[13 \ln(\sqrt{2} + 1) - 23\sqrt{2} + 30] \triangleq .297698157h$$

$$c = \frac{h}{30}[\ln(\sqrt{2} + 1) - 11\sqrt{2} + 15] \triangleq .010834147h$$

$$d = \frac{h}{30}[3 \ln(\sqrt{2} + 1) + 7\sqrt{2} - 10] \triangleq .084787190h$$

$$e = \frac{h}{30}[24 \ln(\sqrt{2} + 1) + 56\sqrt{2} - 80] \triangleq .678297519h$$

$$g = \frac{h}{30}[- 9 \ln(\sqrt{2} + 1) - \sqrt{2} + 10] \triangleq .021780805h.$$

For different point configurations it is often possible to derive formulas of this type. For example, the seven-point formula

$$I = AF(0,0) + B[F(0,\tfrac{h}{2}) + F(\tfrac{h}{2},0)] + C[F(0,h) + F(h,0)] + DF(\tfrac{h}{2},\tfrac{h}{2}) + EF(h,h) \quad (2.14)$$

where

$$A = \frac{h}{12}[5 \ln(1 + \sqrt{2}) + \sqrt{2} - 2] \triangleq .318423458h$$

$$B = \frac{h}{12}[4 \ln(1 + \sqrt{2}) - 12\sqrt{2} + 16] \triangleq .212910967h$$

$$C = \frac{h}{12}[\ln(1 + \sqrt{2}) - 3\sqrt{2} + 4] \triangleq .053227742h$$

$$D = \frac{h}{12}[3 \ln(1 + \sqrt{2}) + 7\sqrt{2} - 10] \triangleq .847871899h$$

$$E = \frac{h}{12}[- 3 \ln(1 + \sqrt{2}) + \sqrt{2} + 2] \triangleq .064174400h,$$

is exact if $F(x,y)$ is any polynomial of the form

$$F(x,y) = c_0 + c_1x + c_2y + c_3xy + c_4x^2 + c_5y^2 + c_6xy^2 + c_7x^2y.$$

From the way the coefficients in formulas (2.13) and (2.14) were obtained, it is obvious that both formulas would give exact results for the test problem of Example 4. A new example is therefore considered:

$$\underline{\text{Example 5}}: \quad I_5 = \int_0^{\frac{1}{4}} \int_0^{\frac{1}{4}} \frac{e^{\sqrt{x^2+y^2}}}{\sqrt{x^2+y^2}} dxdy. \tag{2.15}$$

The integration here can probably not be performed analytically. However, upon changing to polar coordinates, it is found that

$$I_5 = 2 \int_0^{\pi/4} e^{\frac{1}{4}\sec \theta} d\theta - \frac{\pi}{2}, \tag{2.16}$$

and this non-singular integral may be evaluated quite accurately by ordinary Gauss formulas, Simpson's rule, or similar formulas. In Table 2 (on the next page), the results of applying various types of formulas for the numerical evaluation of the integral in (2.15) are listed.

<ins>Comments on the results</ins>: (1) The last case (in which the singularity was ignored) was included merely for comparison. When ordinary Gauss formulas for integration of non-singular integrands are applied like this to the integration of non-negative singular integrands, it often happens that the expected poor "answers" are much too small. (2) Since the function $e^{\sqrt{x^2+y^2}}$ is strongly concave upward, it is to be expected that formula (2.12) (which uses only the four corner points and which assumes the function is linear between them), will give results which are much <ins>too</ins> <ins>large</ins>. The results using this four-point formula are worse than those obtained by using the sixteen-point formula which ignores the singularity. This illustrates the obvious fact that a low

	5-place Value	Error
Correct Value: (obtained by accurate evaluation of the integral in (2.16))	.509626	
4-point process: Cubature formula (2.12)	.52274	.01311
7-point process: Cubature formula (2.14)	.51021	.00058
9-point process: Iterated 3-point Gaussian quadrature assuming logarithmic singularity in the integration with respect to y; (a set-up like formulas (2.4) and (2.5) with lower limit zero)	.50865	-.00098
9-point process: Cubature formula (2.13)	.51081	.00118
16-point process: Iterated 4-point Gaussian quadrature assuming logarithmic singularity in the integration with respect to y; (a set-up like formulas (2.4) and (2.5) with lower limit zero)	.50940	-.00023
16-point process: Cubature formula (II-3) in Appendix II	.51011	.00048
16-point process: Iterated 4-point ordinary Gaussian quadrature ignoring the presence of the singularity completely	.50373	-.00590

Table 2 - Results of Numerical Integration of I_5

order formula should not be used over a large region. Generally, formula (2.12) would only be used in a small region around the singularity; ordinary formulas for evaluation of non-singular integrals may be applied over the remainder of the region. These remarks apply also to somewhat higher order formulas. The meaning of "small region about the singularity" will depend on how widely $F(x,y)$ varies in the region. Intuitively, one asks the question: "May $F(x,y)$ be approximated reasonably well in this region by a polynomial of the degree for which the formula is exact?" (3) The fact that the 7-point cubature formula gave better results than the 9-point cubature formula probably occurred only by chance. (4) In comparing the iterated quadrature methods used in this example with the cubature methods of formulas (2.13) and (II-3) of Appendix II, it should be noted that the following considerations will have a lot to do with the accuracy of the results:

(a) As mentioned before, the Gaussian iterated quadrature method suffers from the fact that near one end of the y-interval, the x integration may be considered to be "near singular", although we go ahead and use ordinary Gaussian quadrature anyway.

(b) Formulas (2.13) and (II-3) are "equally-spaced" formulas, and such formulas do not have the accuracy that generalized Gauss formulas possess; that is, they are not exact for polynomials of as high a degree as is a corresponding Gauss type formula using the same number of points.

For this particular example, it is seen that the iterated quadrature methods turned out to be slightly better than the cubature method in both 9-point and 16-point cases. On the other hand, the cubature formulas (2.14) and (II-3) are somewhat easier to use. This is especially true in the application of the formulas in the numerical solution of integral equations; in this case, a factor in the integrand contains the unknown variable, and it is usually much more convenient to use an equally-spaced formula than one with any other spacing.

§3. Singular integrals of the type

$$I = \int_0^h \int_0^h \ln\sqrt{x^2 + y^2}\, F(x,y)\,dxdy \tag{3.1}$$

Here it is assumed that $F(x,y)$ is analytic in the region

$$0 \le \frac{x}{y} \le h \le \frac{1}{2}\sqrt{2}$$

and that $F(0,0) \ne 0$. In a manner analogous to that used in paragraph 2, equally-spaced cubature formulas may be derived. In Appendix III, four-point, nine-point, and sixteen-point formulas of this type are listed. It is to be noted that the coefficients in these formulas will always be negative if h is in the range $[0,\frac{1}{2}\sqrt{2}]$ which was specified. (Intuitively, one wishes for practical use to rule out any formulas which have some negative and some positive coefficients.)

A good example of a problem of type (3.1) in which $F(x,y)$ is not a polynomial and for which the exact solution is known has eluded the author. In the absence of such a test problem, the following problem was considered:

<u>Example 6</u>: $$J = \int_0^h \int_0^h \ln\sqrt{x^2 + y^2}\, \cos(5xy^2)\,dxdy \tag{3.2}$$

For various values of h, the formulas of Appendix III were tried on this problem. Also, high order iterated Gaussian quadrature (completely ignoring the singularity) was tried. The results of evaluating $-J$ by various formulas are given in Table 3.

	h = 0.1	h = 0.2	h = 0.3	h = 0.5	h = 1.0
4-point formula (III-1)	.02670606	.079085	.1412	.256	.36
9-point formula (III-2)	.02670611	.07909542	.141421	.2635	.3855
16-point formula (III-3)	.02670611	.07909538	.141419	.263395	.3900
9-point formula (ignoring singularity)	.02673	.0792	.1416	.264	.394
64-point formula (ignoring singularity)	.026707	.079099	.14143	.263455	.390973
256-point formula (ignoring singularity)	.02670617	.07909569	.141421	.263437	.390900

Table 3: Results in numerical integration of $-\int_0^h\int_0^h \ln\sqrt{x^2+y^2}\cos(5xy^2)\,dx\,dy$

Comments on the results: (1) Although the exact results are not known, enough work has been done with this problem so that it is felt that we at least know when the "answers" are obviously quite a bit off. For example, then, when it was felt that the "answer" was certainly good to no more than three significant figures, only this many figures were listed in the table. (2) One notes that the three cubature formulas (III-1,2,3) give essentially the same results for $h = 0.1$. For larger values of h, the four-point formula soon begins to give noticeably poorer results. (The function $F(x,y) = \cos(5xy^2)$ cannot be approximated very well in an interval $0 \leq {x \atop y} \leq h$ if h is more than 0.1 or 0.2.) However, the nine-point formula and the sixteen-point formula give quite comparable results for $h = 0.3$. For $h = 1.0$, none of the three cubature formulas should have been used. They were derived assuming $h \leq \frac{1}{2}\sqrt{2}$, and when one uses them for $h = 1.0$, the coefficients in the formula are not of one sign; of course, the weighting function $\ln \sqrt{x^2 + y^2}$ is not always non-positive either if in part of the region $x^2 + y^2 > 1$, (which will happen if $h > \frac{1}{2}\sqrt{2}$). (3) The formulas used to obtain the results in the last three rows of the Table were ordinary Gaussian quadrature formulas applied to both x and y integrations. For example, for the last line, sixteen-point Gauss formulas were used for each quadrature. Instead of our problem, if one were trying to evaluate

$$\int_0^h \int_0^h \cos(5xy^2)\,dx\,dy,$$

even the nine-point formulas would give excellent results for the smaller values of h, and the 64-point and 256-point formulas would have given excellent results for all values of h listed. But when one tries to apply these formulas when the integrand has a singularity, the results (as expected) are not good. For example, for $h = 0.3$, the 256-point formula ignoring the singularity gives the same results as the nine-point cubature formula (III-2).

§4. It is hoped that the preceding examples will cause programmers to look carefully at any integral they wish to evaluate before deciding what integration formula to use on the computer.

Formulas similar to those listed in the three appendices may be derived for many other specific problems. It is certainly possible to set up a machine program for deriving such formulas. Such a program would, however, usually require multiple precision arithmetic. For example, for the sixteen-point cubature formula (II-3), it was necessary to solve ten linear equations for the ten unknown coefficients in the formula, and these equations are quite ill-conditioned. For the four-point formula (II-1), the actual equations were listed earlier in this document (equations (2.11a),(2.11b), and (2.11c)). This particular system is already in triangular form, but it will not be true in general.

From equations (2.11a) - (2.11c), one sees that another difficulty in deriving formulas for specific integration problems might very well be in the evaluation of the integrals analogous to those on the right in equations (2.11a) - (2.11c).

Appendix I

Table of Abscissas and Coefficients in the Generalized Gaussian Formula

$$\int_0^h \ln x \, F(x)dx = \sum_{i=1}^{n} H_i F(x_i)$$

A description of how to derive these formulas is given, for example, in Kopal[1] or Mineur[2]. The function $F(x)$ is assumed to have $2n$ continuous derivatives in $[0,h]$, where $h \leq 1$. The fact that the integral only exists as an improper integral does not have any effect on the method of derivation, but it does limit the choice of methods of deriving simple error expressions.

The basic idea is that the formula

$$\int_0^h \ln x \, F(x)dx = \sum_{i=1}^{n} H_i F(x_i) + R_n \qquad \text{(i)}$$

is derived so that the remainder term R_n is identically zero if $F(x)$ is any polynomial of degree no more than $2n - 1$. In the table below, the proper values of the abscissas x_i and the corresponding coefficients H_i are given for various fixed values of h and n.

The Hermite representation for $F(x)$ in the interval $[0,h]$ using the base points $x_1, x_2, \ldots, x_n$ is (see Steffensen[3])

$$F(x) = \sum_{i=1}^{n} [\ell_i(x)]^2 \{F(x_i)[1 - 2(x - x_i)\ell_i'(x_i)] + (x - x_i)F'(x_i)\}$$

$$+ \frac{F^{(2n)}[\xi(x)]}{(2n)!} \prod_{j=1}^{n} (x - x_j)^2 \qquad \text{(ii)}$$

where

$$\ell_i(x) = \prod_{\substack{k=1 \\ (k\neq i)}}^{n} \frac{(x - x_k)}{(x_i - x_k)}$$

and where $0 < \xi(x) < h$.

Since the sum in equation (ii) (which will be designated as $Q_{2n-1}(x)$) is merely a polynomial of degree $2n - 1$, and since $F(x)$ is continuous, it follows that $F^{(2n)}[\xi(x)]$ is a continuous function of x. Substitution of equation (ii) into (i) then gives an expression for R_n:

$$R_n = \int_0^h \ln x \, Q_{2n-1}(x)dx + \int_0^h \ln x \, \frac{F^{(2n)}[\xi(x)]}{(2n)!} \prod_{j=1}^{n} (x - x_j)^2 dx$$

$$- \sum_{i=1}^{n} H_i Q_{2n-1}(x_i) - \sum_{i=1}^{n} H_i \frac{F^{(2n)}[\xi(x_i)]}{(2n)!} \prod_{j=1}^{n} (x_i - x_j)^2.$$

The product in the last term is zero; the first integral is equal to the first sum because the formula was originally derived to be exact for polynomials of degree $(2n - 1)$ or less. Thus

$$R_n = \int_0^h \ln x \, \frac{F^{(2n)}[\xi(x)]}{(2n)!} \prod_{j=1}^{n} (x - x_j)^2 dx.$$

Since $F^{(2n)}[\xi(x)]$ is continuous and since the other factor in the integrand is always negative, one may use the mean value theorems applied to the improper integral to obtain the formula

$$R_n = \frac{F^{(2n)}(\zeta)}{(2n)!} \int_0^h \ln x \prod_{j=1}^{n} (x - x_j)^2 dx$$

where $0 \leq \zeta \leq h$. The integration here may be carried out in closed form, and for any particular values of h and n a numerical value of the coefficient of $F^{(2n)}(\zeta)$ could be obtained if desired.

Abscissas and coefficients for the formulas are given in the following tables.

$$\int_0^h \ln x\, F(x)dx = \sum_{i=1}^{n} H_i F(x_i)$$

	Two-point formulas x_i	Two-point formulas H_i	Three-point formulas x_i	Three-point formulas H_i
h = .1	.017 065 3648	-.188 936 512	.009 038 5371	-.117 704 182
	.076 340 9457	-.141 321 998	.046 848 5242	-.139 364 134
			.087 717 3234	-.073 190 193
h = .2	.032 526 740	-.309 155 272	.017 311 2632	-.197 105 695
	.151 048 729	-.212 732 310	.092 032 2473	-.217 367 372
			.174 760 3835	-.107 414 515
h = .25	.039 827 506	-.358 810 887	.021 252 272	-.230 944 257
	.187 818 171	-.237 762 703	.114 098 280	-.247 084 847
			.218 033 359	-.118 544 486
h = .3	.046 866 292	-.403 476 458	.025 076 930	-.261 970 538
	.224 159 419	-.257 715 384	.135 810 533	-.272 407 593
			.261 119 549	-.126 813 710
h = .4	.060 185 480	-.480 899 476	.032 395 246	-.317 275 288
	.295 361 084	-.285 616 817	.178 113 942	-.312 698 376
			.346 625 133	-.136 542 629
h = .5	.072 495 937	-.545 589 256	.039 281 165	-.365 307 501
	.364 106 635	-.300 984 334	.218 757 540	-.342 191 529
			.430 968 225	-.139 074 559
h = .75	.098 332 529	-.664 069 402	.054 430 334	-.460 263 416
	.517 865 507	-.301 692 152	.310 616 188	-.382 620 062
			.631 807 628	-.122 878 077
h = 1.0	.112 008 806	-.718 539 319	.063 890 793	-.513 404 552
	.602 276 908	-.281 460 681	.368 997 064	-.391 980 041
			.766 880 304	-.094 615 407

$$\int_0^h \ln x \, F(x)dx = \sum_{i=1}^{n} H_i F(x_i)$$

	Four-point Formulas x_i	Four-point Formulas H_i	Five-point Formulas x_i	Five-point Formulas H_i
	.005 579 3787	-.080 432 5170	.003 785 3873	-.058 679 2293
	.030 456 8106	-.112 913 0245	.021 146 0155	-.090 010 3886
h = .1	.065 083 2445	-.092 721 2481	.048 016 9933	-.087 763 4421
	.092 564 6649	-.044 191 7197	.075 741 5540	-.064 349 1963
			.095 035 7147	-.029 456 2529
	.010 730 0607	-.136 781 961	.007 303 6269	-.100 898 343
	.059 732 9846	-.180 961 542	.041 473 7959	-.147 093 364
h = .2	.129 046 5053	-.140 154 911	.094 989 2687	-.136 215 523
	.184 800 1041	-.063 989 169	.150 759 6325	-.095 367 634
			.189 888 8128	-.042 312 718
	.013 199 0687	-.161 254 261	.008 997 7473	-.119 469 913
	.074 022 3111	-.208 196 736	.051 405 8244	-.170 641 071
h = .25	.160 649 9113	-.156 984 793	.118 143 6743	-.154 482 727
	.230 795 6060	-.070 137 800	.188 016 1836	-.105 790 569
			.237 247 4844	-.046 189 311
	.015 605 5281	-.183 944 963	.010 653 955	-.136 818 022
	.088 086 1632	-.232 212 713	.061 191 357	-.191 814 948
h = .3	.191 986 7991	-.170 544 383	.141 073 659	-.169 924 693
	.276 698 6323	-.074 489 782	.225 090 424	-.113 791 218
			.284 554 707	-.048 842 960
	.020 242 153	-.225 038 822	.013 860 195	-.168 565 160
	.115 524 836	-.272 635 015	.080 323 520	-.228 532 902
h = .4	.253 774 725	-.189 937 617	.186 217 509	-.194 139 340
	.368 171 418	-.078 904 839	.298 616 333	-.124 050 550
			.378 983 205	-.051 228 341
	.024 650 669	-.261 493 609	.016 929 963	-.197 115 290
	.141 985 961	-.305 065 815	.098 846 742	-.259 304 126
h = .5	.314 166 312	-.201 254 116	.230 289 847	-.211 378 918
	.459 053 527	-.078 760 050	.371 122 736	-.128 274 873
			.473 080 262	-.050 500 383
	.034 597 958	-.336 501 008	.023 968 326	-.257 348 518
	.202 794 754	-.360 747 058	.141 941 301	-.316 979 130
h = .75	.455 812 835	-.204 766 138	.334 012 731	-.232 815 086
	.680 823 438	-.063 747 351	.544 908 302	-.120 066 808
			.705 185 931	-.038 552 012
	.041 448 480	-.383 464 068	.029 134 472	-.297 893 472
	.245 274 914	-.386 875 318	.173 977 213	-.349 776 227
h = 1.0	.556 165 454	-.190 435 127	.411 702 520	-.234 488 290
	.848 982 395	-.039 225 487	.677 314 175	-.098 930 459
			.894 771 361	-.018 911 552

$$\int_0^h \ln x \, F(x)dx = \sum_{i=1}^{n} H_i F(x_i)$$

	Six-point Formulas x_i	Six-point Formulas H_i	Seven-point Formulas x_i	Seven-point Formulas H_i
	.002 737 2522	-.044 867 1463	.002 072 1068	-.035 527 6951
	.015 469 6555	-.072 651 9894	.011 784 1174	-.059 663 9342
	.036 303 1065	-.077 680 9568	.028 206 4839	-.067 568 1217
h = .1	.060 487 2300	-.067 222 4997	.048 553 9795	-.063 982 2229
	.082 296 5498	-.046 834 4688	.069 244 2584	-.032 329 9697
	.096 456 8465	-.021 001 4482	.086 559 5443	-.035 470 0086
			.097 346 5800	-.015 716 5571
	.005 295 0647	-.077 799 6177	.004 016 8810	-.062 016 4469
	.030 357 5278	-.120 458 4218	.023 141 2079	-.100 038 5777
	.071 748 1227	-.123 092 4025	.055 729 0893	-.108 818 0112
h = .2	.120 160 3044	-.102 007 6953	.096 347 1971	-.099 062 9590
	.164 114 1637	-.068 577 9746	.137 872 9565	-.078 139 9389
	.192 802 6065	-.030 011 4705	.172 790 5153	-.051 433 2069
			.194 620 7986	-.022 378 4418
	.006 530 9449	-.092 422 0578	.004 959 0934	-.073 862 5772
	.037 641 3068	-.140 584 7603	.028 704 7253	-.117 287 7392
	.089 209 6762	-.140 908 2984	.069 288 9353	-.125 452 0207
h = .25	.149 727 1075	-.114 469 7378	.120 001 7469	-.112 217 0601
	.204 852 8015	-.075 514 5934	.171 977 8038	-.087 005 2591
	.240 934 2157	-.032 674 1424	.215 788 0211	-.056 429 8697
			.243 231 0509	-.024 319 0640
	.007 741 8903	-.106 154 737	.005 883 9101	-.085 033 5373
	.044 825 428	-.158 911 943	.034 197 4598	-.133 134 9773
	.106 499 312	-.156 404 554	.082 718 5014	-.140 190 7592
h = .3	.179 106 115	-.124 589 891	.143 492 1782	-.123 289 2070
	.245 466 855	-.080 676 771	.205 933 9771	-.093 948 6461
	.289 034 540	-.034 453 945	.258 698 4269	-.060 001 0805
			.291 820 9534	-.025 593 6338
	.010 094 293	-.131 473 543	.007 685 2608	-.105 745 899
	.058 898 892	-.191 288 667	.044 975 476	-.161 490 108
	.140 543 490	-.181 914 363	.109 178 862	-.165 181 407
h = .4	.237 247 089	-.139 293 045	.189 947 832	-.140 512 231
	.326 262 632	-.086 642 714	.273 347 751	-.103 282 880
	.385 122 046	-.035 903 961	.344 213 964	-.063 752 179
			.388 927 180	-.026 551 589
	.012 357 848	-.154 463 257	.009 425 1483	-.124 689 545
	.072 569 130	-.219 128 433	.055 472 574	-.186 293 354
	.173 810 761	-.201 672 708	.135 071 476	-.185 450 850
h = .5	.294 428 876	-.148 195 050	.235 614 042	-.152 577 010
	.406 333 465	-.088 009 317	.339 964 610	-.107 834 450
	.481 007 530	-.035 104 825	.429 209 778	-.063 915 195
			.485 902 001	-.025 813 186

$$\int_0^h \ln x \, F(x)dx = \sum_{i=1}^{n} H_i F(x_i)$$

	Six-point Formulas		Seven-point Formulas	
	x_i	H_i	x_i	H_i
	.017 606 007	-.203 816 913	.013 492 725	-.165 885 575
	.104 662 873	-.273 867 828	.080 287 312	-.236 580 830
	.252 541 235	-.232 953 197	.196 665 459	-.221 087 185
h = .75	.431 126 864	-.152 443 361	.344 963 158	-.166 619 048
	.600 829 037	-.076 930 220	.500 964 878	-.104 280 334
	.718 785 844	-.025 750 035	.637 433 036	-.052 901 605
			.727 073 965	-.018 406 978
	.021 634 006	-.238 763 663	.016 719 355	-.196 169 389
	.129 583 391	-.308 286 573	.100 185 678	-.270 302 644
	.314 020 450	-.245 317 427	.246 294 246	-.239 681 873
h = 1.0	.538 657 217	-.142 008 757	.433 463 493	-.165 775 775
	.756 915 337	-.055 454 622	.632 350 988	-.088 943 227
	.922 668 851	-.010 168 959	.811 118 627	-.033 194 304
			.940 848 167	-.005 932 7870

Eight-point Formulas

	.001 623 6190	-.028 901 5876
	.009 265 6696	-.049 825 3739
	.022 462 9083	-.058 678 5672
h = .1	.039 487 9968	-.058 818 6615
	.058 025 2058	-.052 495 3423
	.075 504 4191	-.041 603 7363
	.089 469 1394	-.027 737 3689
	.097 939 6237	-.012 197 8715
	.003 153 0217	-.050 725 2236
	.018 208 5251	-.084 294 1729
	.044 381 3184	-.095 731 6168
h = .2	.078 310 8566	-.092 590 0626
	.115 415 5869	-.079 862 3292
	.150 543 2585	-.061 395 6310
	.178 704 9274	-.039 965 9145
	.195 829 5772	-.017 322 6319
	.003 895 6151	-.060 541 1921
	.022 594 4803	-.099 185 5690
	.055 184 0243	-.110 975 3784
h = .25	.097 517 2457	-.105 675 7286
	.143 902 4230	-.089 725 6908
	.187 901 3513	-.067 964 3671
	.223 238 4836	-.043 706 0875
	.244 756 1390	-.018 799 5766

$$\int_0^h \ln x\, F(x)dx = \sum_{i=1}^{n} H_i F(x_i)$$

Eight-point Formulas

	x_i	H_i
	.004 625 5195	-.069 827 8231
	.026 928 2927	-.112 957 6094
	.065 886 9117	-.124 658 4226
h = .3	.116 587 3281	-.116 957 3535
	.172 245 0299	-.097 773 8166
	.225 143 4404	-.072 948 1768
	.267 709 4464	-.046 311 9302
	.293 668 7565	-.019 756 7089
	.006 050 2310	-.087 123 271
	.035 444 175	-.137 831 802
	.086 990 833	-.148 324 262
h = .4	.154 299 396	-.135 253 690
	.228 458 891	-.109 574 963
	.299 232 903	-.079 155 968
	.356 430 573	-.048 822 802
	.391 443 600	-.020 429 534
	.007 430 4341	-.103 031 774
	.043 756 172	-.159 860 455
	.107 670 933	-.168 086 490
h = .5	.191 382 639	-.149 070 658
	.283 944 674	-.116 869 081
	.372 678 364	-.081 404 215
	.444 772 010	-.048 471 625
	.489 128 485	-.019 779 292
	.010 677 906	-.137 975 753
	.063 512 116	-.205 495 866
	.157 081 786	-.204 954 207
h = .75	.280 413 715	-.169 505 437
	.417 959 377	-.121 017 820
	.551 576 813	-.074 576 282
	.662 404 789	-.038 421 023
	.732 473 320	-.013 815 167
	.013 320 244	-.164 416 605
	.079 750 429	-.237 525 610
	.197 871 029	-.226 841 984
h = 1.0	.354 153 994	-.175 754 079
	.529 458 575	-.112 924 030
	.701 814 530	-.057 872 211
	.849 379 320	-.020 979 074
	.953 326 450	-.003 686 4071

Appendix II

Cubature Formulas for $I = \int_0^h \int_0^h \frac{F(x,y)}{\sqrt{x^2 + y^2}} dxdy$ where $0 < h < \frac{1}{2}\sqrt{2}$

Four Point Formula

$I = a_1 F(0,0) + a_2[F(h,0) + F(0,h)] + a_3 F(h,h)$ where

$$a_1 = \frac{h}{3}[3 \ln(1 + \sqrt{2}) - \sqrt{2} + 1] = .743\ 302\ 400h$$

$$a_2 = \frac{h}{6}[3 \ln(1 + \sqrt{2}) - \sqrt{2} + 1] = .371\ 651\ 200h \qquad \text{(II-1)}$$

$$a_3 = \frac{2h}{3}(\sqrt{2} - 1) = .276\ 142\ 375h$$

The above formula is exact if $F(x,y)$ is any polynomial of the form $c_0 + c_1 x + c_2 y + c_3 xy$.

Nine Point Formula

$$I = a_1 F(0,0) + a_2[F(\tfrac{h}{2},0) + F(0,\tfrac{h}{2})] + a_3[F(h,0) + F(0,h)]$$
$$+ a_4 F(\tfrac{h}{2},\tfrac{h}{2}) + a_5[F(h,\tfrac{h}{2}) + F(\tfrac{h}{2},h)] + a_6 F(h,h)$$

where (when $L = \frac{h}{30} \ln(1 + \sqrt{2})$ and when $S = \frac{\sqrt{2}\,h}{30}$ and when $K = \frac{h}{6}$)

$$a_1 = 11L - S = .2760\ 29863h$$

$$a_2 = 13L - 23S + 6K = .2976\ 98157h$$

$$a_3 = L - 11S + 3K = .0108\ 34147h \qquad \text{(II-2)}$$

$$a_4 = 24L + 56S - 16K = .6782\ 97519h$$

$$a_5 = 3L + 7S - 2K = .0847\ 87190h$$

$$a_6 = -9L - S + 2K = .0217\ 80805h$$

The above formula is exact if $F(x,y)$ is any polynomial of the form $c_0 + c_1 x + c_2 x^2 + c_3 y + c_4 xy + c_5 x^2 y + c_6 y^2 + c_7 xy^2 + c_8 x^2 y^2$.

Appendix III

Cubature Formulas for $I = \int_0^h \int_0^h F(x,y) \ln\sqrt{x^2 + y^2}\, dxdy$ where $0 < h < \frac{1}{2}\sqrt{2}$

Four Point Formula

$I = a_1 F(0,0) + a_2[F(h,0) + F(0,h)] + a_3 F(h,h)$ where

$$\begin{aligned}
a_1 &= \frac{h^2}{48}[12 \ln h + 4 \ln 2 + 4\pi - 25] = h^2[\tfrac{1}{4} \ln h - .201\ 271\ 680] \\
a_2 &= \frac{h^2}{48}[12 \ln h + 4 \ln 2 + 4\pi - 19] = h^2[\tfrac{1}{4} \ln h - .076\ 271\ 680] \\
a_3 &= \frac{h^2}{48}[12 \ln h + 12 \ln 2 \qquad - 9] = h^2[\tfrac{1}{4} \ln h - .014\ 213\ 205]
\end{aligned} \tag{III-1}$$

The above formula is exact if $F(x,y)$ is any polynomial of the form $c_0 + c_1 x + c_2 y + c_3 xy$.

Nine Point Formula

$$I = a_1 F(0,0) + a_2[F(\tfrac{h}{2},0) + F(0,\tfrac{h}{2})] + a_3[F(h,0) + F(0,h)]$$
$$+ a_4 F(\tfrac{h}{2},\tfrac{h}{2}) + a_5[F(h,\tfrac{h}{2}) + F(\tfrac{h}{2},h)] + a_6 F(h,h)$$

where (when $H^* = \frac{h^2 \ln h}{36}$ and $L = \frac{h^2 \ln 2}{180}$ and $P = \frac{\pi h^2}{360}$ and $K = \frac{h^2}{720}$)

$$\begin{aligned}
a_1 &= H^* + 7L + 2P - 79K &&= h^2[\tfrac{1}{36} \ln h - .065\ 313\ 206] \\
a_2 &= 4H^* - 20L + 20P - 140K &&= h^2[\tfrac{1}{9} \ln h - .096\ 927\ 873] \\
a_3 &= H^* - 17L + 8P - K &&= h^2[\tfrac{1}{36} \ln h + .002\ 960\ 3808] \\
a_4 &= 16H^* + 112L + 32P - 624K &&= h^2[\tfrac{4}{9} \ln h - .156\ 122\ 407] \\
a_5 &= 4H^* + 28L + 8P - 116K &&= h^2[\tfrac{1}{9} \ln h + .016\ 524\ 954] \\
a_6 &= H^* - 11L - 16P + 137K &&= h^2[\tfrac{1}{36} \ln h + .008\ 292\ 4433]
\end{aligned} \tag{III-2}$$

The above formula is exact is $F(x,y)$ is any polynomial of the form $c_0 + c_1 x + c_2 x^2 + c_3 y + c_4 xy + c_5 x^2 y + c_6 y^2 + c_7 xy^2 + c_8 x^2 y^2$.

Appendix II (continued)

Cubature Formulas for $I = \int_0^h \int_0^h \frac{F(x,y)}{\sqrt{x^2 + y^2}} dxdy$ where $0 < h < \frac{1}{2}\sqrt{2}$

Sixteen Point Formula

$$I = a_1F(0,0) + a_2[F(\tfrac{h}{3},0) + F(0,\tfrac{h}{3})] + a_3[F(\tfrac{2h}{3},0) + F(0,\tfrac{2h}{3})]$$
$$+ a_4[F(h,0) + F(0,h)] + a_5F(\tfrac{h}{3},\tfrac{h}{3}) + a_6[F(\tfrac{2h}{3},\tfrac{h}{3}) + F(\tfrac{h}{3},\tfrac{2h}{3})]$$
$$+ a_7[F(h,\tfrac{h}{3}) + F(\tfrac{h}{3},h)] + a_8F(\tfrac{2h}{3},\tfrac{2h}{3}) + a_9[F(h,\tfrac{2h}{3}) + F(\tfrac{2h}{3},h)]$$
$$+ a_{10}F(h,h)$$

where (when $L = \frac{h \ln(1 + \sqrt{2})}{160}$ and $S = \frac{h\sqrt{2}}{3360}$ and $K = \frac{h}{1680}$)

$$a_1 = 28L - 292S + 236K = .171\ 814\ 675h$$
$$a_2 = 75L - 1413S + 657K = .209\ 487\ 987h$$
$$a_3 = -\ 114L - 1170S + 1926K = .026\ 000\ 525h \qquad \text{(II-3)}$$
$$a_4 = -\ 49L - 65S + 541K = .024\ 744\ 850h$$
$$a_5 = 5184S - 2916K = .446\ 215\ 211h$$
$$a_6 = 405L - 3483S - 1053K = .138\ 207\ 298h$$
$$a_7 = 180L - 1548S - 468K = .061\ 425\ 466h$$
$$a_8 = -\ 648L + 9720S - 648K = .135\ 840\ 492h$$
$$a_9 = -\ 63L + 1233S - 225K = .037\ 996\ 448h$$
$$a_{10} = 72L - 1720S + 572K = .013\ 151\ 648h$$

The above formula is exact if $F(x,y)$ is any polynomial of the form

$$c_0 + c_1x + c_2x^2 + c_3x^3 + c_4y + c_5xy + c_6x^2y + c_7x^3y + c_8y^2 + c_9xy^2$$
$$+ c_{10}x^2y^2 + c_{11}x^3y^2 + c_{12}y^3 + c_{13}xy^3 + c_{14}x^2y^3 + c_{15}x^3y^3.$$

Appendix III (continued)

Cubature Formulas for $I = \int_0^h \int_0^h F(x,y) \ln\sqrt{x^2+y^2}\,dxdy$ where $0 < h < \frac{1}{2}\sqrt{2}$

Sixteen Point Formulas

$$I = a_1F(0,0) + a_2[F(\tfrac{h}{3},0) + F(0,\tfrac{h}{3})] + a_3[F(\tfrac{2h}{3},0) + F(0,\tfrac{2h}{3})]$$
$$+ a_4[F(h,0) + F(0,h)] + a_5F(\tfrac{h}{3},\tfrac{h}{3}) + a_6[F(\tfrac{2h}{3},\tfrac{h}{3}) + F(\tfrac{h}{3},\tfrac{2h}{3})]$$
$$+ a_7[F(h,\tfrac{h}{3}) + F(\tfrac{h}{3},h)] + a_8F(\tfrac{2h}{3},\tfrac{2h}{3}) + a_9[F(h,\tfrac{2h}{3}) + F(\tfrac{2h}{3},h)] + a_{10}F(h,h)$$

where (when $H^* = \frac{h^2 \ln h}{64}$ and $L = \frac{h^2 \ln 2}{1680}$ and $P = \frac{h^2\pi}{1680}$ and $K = \frac{h^2}{53760}$)

$$a_1 = H^* - 13L - 4P - 967K = h^2[\tfrac{1}{64}\ln h - .030\,830\,973]$$
$$a_2 = 3H^* + 27L + 81P - 12207K = h^2[\tfrac{3}{64}\ln h - .064\,455\,221]$$
$$a_3 = 3H^* - 351L - 108P + 18411K = h^2[\tfrac{3}{64}\ln h - .004\,311\,2601]$$
$$a_4 = H^* - 139L - 67P + 9659K = h^2[\tfrac{1}{64}\ln h - .002\,970\,4856]$$
$$a_5 = 9H^* + 270L - 135P - 1215K = h^2[\tfrac{9}{64}\ln h - .163\,651\,202]$$
$$a_6 = 9H^* + 513L + 594P - 72333K = h^2[\tfrac{9}{64}\ln h - .023\,045\,066] \qquad \text{(III-3)}$$
$$a_7 = 3H^* + 198L + 279P - 32853K = h^2[\tfrac{3}{64}\ln h - .007\,683\,7845]$$
$$a_8 = 9H^* + 27L - 864P + 86913K = h^2[\tfrac{9}{64}\ln h + .012\,148\,911]$$
$$a_9 = 3H^* + 63L - 126P + 11697K = h^2[\tfrac{3}{64}\ln h + .007\,951\,6953]$$
$$a_{10} = H^* - 66L + 117P - 10119K = h^2[\tfrac{1}{64}\ln h + .003\,333\,2599]$$

The above formula is exact if $F(x,y)$ is any polynomial of the form

$$c_0 + c_1x + c_2x^2 + c_3x^3 + c_4y + c_5xy + c_6x^2y + c_7x^3y + c_8y^2 + c_9xy^2$$
$$+ c_{10}x^2y^2 + c_{11}x^3y^2 + c_{12}y^3 + c_{13}xy^3 + c_{14}x^2y^3 + c_{15}x^3y^3.$$

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